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SMILES ClO + HO2 HOCl + O2
Estimation of the reaction rate constant of ClO + HO2 to HOCl + O2 by SMILES observation

[1*], [2], [1], [2]
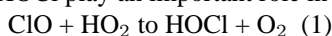KURIBAYASHI, Kouta[1*], SAGAWA, Hideo[2], SATO, Tomohiro[1], KASAI, YASUKO[2]

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HOCl play an important role in the ozone chemistry to link the odd ClOx and the odd HOx with the reaction,

$ClO + HO_2$ to $HOCl + O_2$ (1)

This is the only one reaction to produce HOCl in the middle atmosphere in the gas phase. This reaction is a key in the middle stratospheric ozone loss for the partitioning of the Cl atomic radical.

There are several laboratory studies to determine the reaction rate constant of (1). But these reaction rate constants have large discrepancies with large uncertainties as $k_{HOCl} = 3.3*10^{-11}\exp(-850/T) + 4.5*10^{-12}(T/300)^{-3.7}$ (Stimpfle et al, 1979) or $k_{HOCl} = (1.75+-0.52)*10^{-12}\exp[(368+-78)/T]$ (Hickson et al, 2007). Main reason for its uncertainty is that the chemical reaction of (1) is the reaction of ClO radical and HO_2 radical. Therefore, in laboratory experiment for the calculation of this reaction rate constant, the generations of two radical is too difficult, and it is also difficult to extract only this reaction purely.

We have estimated the reaction rate constant of (1) from the atmospheric observation directly in the upper stratosphere/ lower mesosphere (US/LM) region by using a new super-sensitive remote sensing technology named Superconducting SubMillimeter-wave Limb Emission Sounder (SMILES) on the International Space Station (ISS)

We had estimate the reaction rate constant of (1) with the procedure as below.

1) We discovered that the time period when the reaction of (1) was purely happened is from one hour after sunset to one hour before sunrise.

2) From the time variations of ClO and HO_2 of this time period, we calculated the reaction rate constant of (1). The estimated reaction rate constant is $8.9*10^{-12}$ [cm^3 molecule^{-1} s^{-1}] (20S-40S, 0.54hPa, 254.5K)

3) From this reaction rate constant and the time variations of ClO and HO_2, we calculated the time variations of HOCl.

4) We checked the comparison between these calculated values and observed values. Our calculated values was in good agreement with the observed values.

5) We checked the comparison between our estimated reaction rate constants and the previous reaction rate constants. Our estimated reaction rate constant, $k_{HOCl} = 8.9*10^{-12}$ (20S-40S, 0.54hPa, 254.5K), was between the reaction rate constant, $k_{HOCl} = 7.43*10^{-12}$ (Hickson et al), and the reaction rate constant, $k_{HOCl} = 9.44*10^{-12}$ (Stimpfle et al).

: , SMILES, HOCl
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